Final Report
AASERT Supplement

Modeling of Plasma Remediation of NO from Diesel Exhaust for Military Engines

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Submitted to:

Dr. Gabriel Roy
Office of Naval Research
Code 1132P
800 N. Quincy St.
Arlington, VA 22217-5000

Submitted by:

Prof. Mark J. Kushner
University of Illinois
Department of Electrical and Computer Engineering
1406 W. Green St.
Urbana, IL 61801
(217) 244-5137 FAX: (217) 244-7097
e-mail: mjk@uiuc.edu

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6. AUTHOR(S)
Mark J. Kushner

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
University of Illinois at Urbana-Champaign
Department of Electrical & Computer Engineering
1406 W. Green St.
Urbana, IL 61801

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800 N. Quincy St.
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13. ABSTRACT (Maximum 200 words)
Plasma remediation is a technique whereby toxins in atmospheric pressure gas streams can be treated or removed. In this research project computer models for plasma remediation of NOx and volatile organic compounds (VOCs) from air streams have been developed and parameterized. The goals of this project are to determine the dominant reaction mechanisms and to propose methods to optimize the energy efficiency of the process.

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I. Description of Research Goals

The emission of N_xO_y (oxides of nitrogen) from diesel engine exhaust is an acknowledged environmental problem in both the civilian and military sectors. Recently enacted legislation will reduce the allowable emission levels of N_xO_y by more than a factor of 5 for civilian on-road vehicles and stationary sources during next 3 years. The high probability that military engines will be held to the same standards has motivated research into energy efficient methods to reduce these emissions which will not detrimentally affect their battle preparedness.

In this program of research, computer models were developed to investigate the plasma remediation of N_xO_y from diesel engine exhaust and remediation of volatile organic compounds (VOCs) from a variety of sources. The goals of this work were to both investigate the dominant physical processes which control the plasma remediation and to develop physics based design models to optimize the process. The plasma reactors of interest were dominantly dielectric barrier discharges (DBDs). We have also investigated low pressure plasma material processing reactors which are sources of green house gases such as CFCs and PFCs. This work was performed in parallel with a project funded by the Semiconductor Research Corp.

The research performed under this AASERT grant supplemented the work performed under the ONR grant "Modeling Studies of Pulsed Power Plasma Devices" Contract N00014-90-J-1967, and is summarized in the final report for that contract. Reprints of articles refereed to here can also be found that final report.

(Note: References will be made to publications listed in Sections III and IV.

TH refers to "Theses"
JA refers to "Journal Articles"
IPP refers to "Invited Conference and Workshop Presentations with Proceedings"
CPP refers to "Contributed Conference and Workshop Presentations with Proceedings"
CPA refers to "Contributed Conference and Workshop Presentations with Abstracts")

II. Overview of Results

We initially investigated the plasma chemistry of NO_x remediation from humid air **(TH-1, JA-4,6; IPP-8)**. We determined the dominant reaction pathways and determined the conditions whereby the energy required for remediation can be minimized. We also investigated reaction pathways for plasma remediation of select VOCs **(TH-1, JA-3)**. In the next phase of work, we turned our attention to the filamentary nature of the plasma in DBDs. The plasma density and gas heating rates are large in the core of the microstreamers. The scaling characteristics and energy efficiency of toxic gas remediation will therefore depend on power deposition and plasma hydrodynamics occurring in the microstreamers. These phenomena, and their impact on the plasma chemistry were investigated with 1-dimensional models **(TH-1, JA-5, IPP-9, CPP-10, CPA-11)**. In this work, we quantified the decrease in remediation efficiency

resulting from gas heating in the core of the streamer and quantified the consequences of interactions between closely spaced microstreamers.

During the past year, we turned our attention to development of low pressure plasma sources as used in semiconductor material processing. The goals of this work were to address emission of CFCs and PFCs, which are greenhouse gases, by these plasma sources and to develop a modeling infrastructure which can used to design reactors which have a minimum of such emissions. AASERT funding was used to leverage funding from the Semiconductor Research Corp. to finalize model modifications which are enabling us to investigate low CFC emitting plasma etching reactors (**TH-2, JA-7**). That work is now continuing under other funding.

III. Personnel Supported

The following students have were supported by this ASSERT.

Person	Position/Degree Received	Status Upon Leaving the University of Illinois
Ann C. Gentile	Graduate Student Ph.D. Chemical Physics	Postdoctoral Research Fellow Sandia National Labs Livermore CA
Jeff Yang	Graduate Student Electrical and Computer Engineering	
Michael J. Grapperhaus	Graduate Student Ph.D. Nuclear Engineering	R&D Engineer Materials Research Corp. Phoenix, AZ
Ronald Kinder	Graduate Student Nuclear Engineering	

IV. Publications, Presentations and Theses Citing Support by the ASSERT (or the Parent Grant during the ASSERT period)

A. Theses (TH)

1. A. C. Gentile, "Kinetic Processes and Plasma Remediation of Toxic Gases", Ph.D. Thesis, University of Illinois, 1995.
2. M. J. Grapperhaus, "Multiscale Transport Phenomena in Low Pressure Plasmas", Ph.D., University of Illinois, 1997.

B. Journal Articles (JA)

3. A. C. Gentile and M. J. Kushner, "Plasma Remediation of Perchloroethylene (PCE) in Humid Gas Streams", J. Appl. Phys. 78, 2977 (1995)

4. A. C. Gentile and M. J. Kushner "Reaction Chemistry and Optimization of Plasma Remediation of N_xO_y from Gas Streams", J. Appl. Phys. 78, 2074 (1995)

5. A. C. Gentile and M. J. Kushner, "Microstreamer Dynamics During Plasma Remediation of N_xO_y in Dielectric Barrier Discharges", J. Appl. Phys. 79, 3877 (1996)

6. A. C. Gentile and M. J. Kushner, "The Effect of CO_2 on the Plasma Remediation of N_xO_y", Appl. Phys. Lett. 68, 2064 (1996)

7. M. J. Grapperhaus, Z. Krivokapic and M. J. Kushner, "Design Issues in Ionized Metal Physical Vapor Deposition of Copper", to be published in J. Appl. Phys., 1 December 1997.

C. Invited Conference and Workshop Presentations with Proceedings (IPP)

8. M. J. Kushner and A. C. Gentile, "Modeling of Plasma Remediation of SO_2, N_xO_y and VOCs: Progress Report and Databases", Workshop on the Treatment of Gaseous Emissions via Plasma Technology, NIST, Gaithersburg, MD, March 1995.

9. A. C. Gentile, J. Yang and M. J. Kushner, "Microstreamer Initiated Advection in Dielectric Barrier Discharges for Plasma Remediation of N_xO_y: Single and Multiple Streamers", 1995 Diesel Emissions Research Workshop, Department of Energy, La Jolla, CA, July 1995.

D. Contributed Conference and Workshop Presentations with Proceedings (CPP)

10. A. C. Gentile, and M. J. Kushner, "Microstreamer Dynamics During Plasma Remediation of NO Using Atmospheric Pressure Dielectric Barrier Discharges: Single and Multiple Streamers", Proceedings of the 8th ONR Propulsion Program Annual Meeting, La Jolla, CA, October 1995.

E. Contributed Conference Presentations with Abstracts Only (CPA)

11. A. C. Gentile, J. Yang and M. J. Kushner, "Streamer Dynamics in Dielectric Barrier Discharges for Plasma Remediation of SO_x/N_xO_y: Single and Multiple Streamers", 48th Gaseous Electronics Conference, Berkeley, CA, October 1995 (Bull. Am. Phys. Soc. 40, 1587 (1995))